Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 09:53 PM JST

PDB ID	:	6JW1
Title	:	Universal RVD R* accommodates 5mC via water-mediated interactions
Authors	:	Liu, L.; Yi, C.
Deposited on	:	2019-04-18
Resolution	:	2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

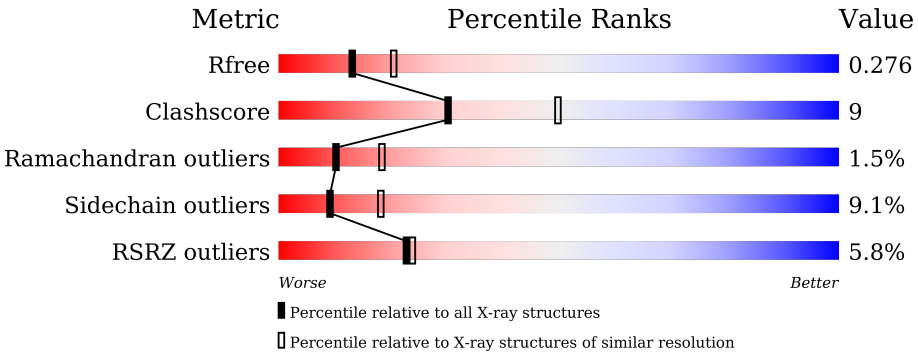
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	5% 82% 14% ·
1	B	498	7% 79% 15% 5% ·
2	C	17	6% 76% 18% 6%
2	I	17	6% 65% 24% 12%
3	D	17	6% 76% 18% 6%
3	J	17	6% 71% 29%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TAL effector.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3606	2253	675	666	12			
1	B	496	Total	C	N	O	S	0	0	0
			3601	2250	673	666	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			336	163	50	107	16			
2	C	17	Total	C	N	O	P	0	0	0
			336	163	50	107	16			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	D	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	I	4	Total	O	0	0
			4	4		
4	B	9	Total	O	0	0
			9	9		

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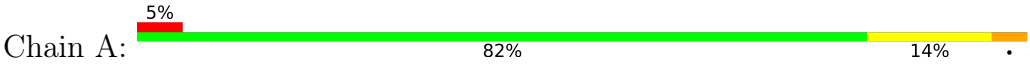
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0

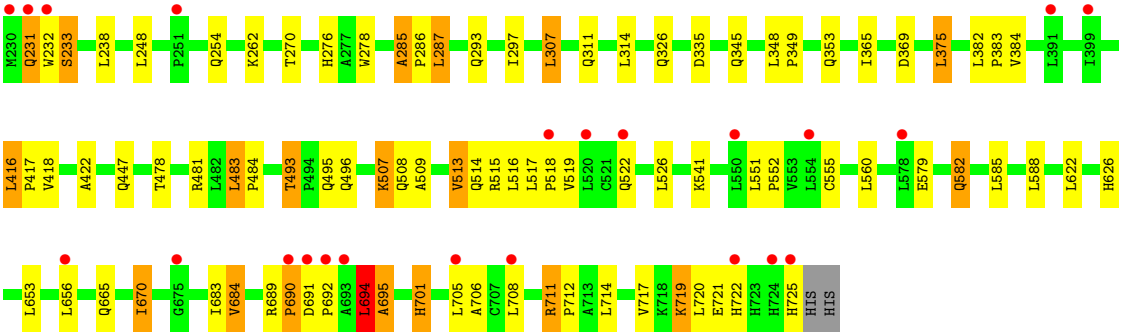
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TAL effector

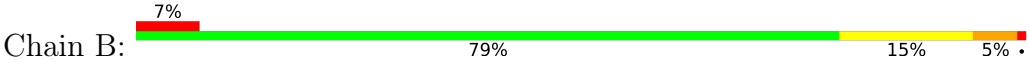
Chain A:

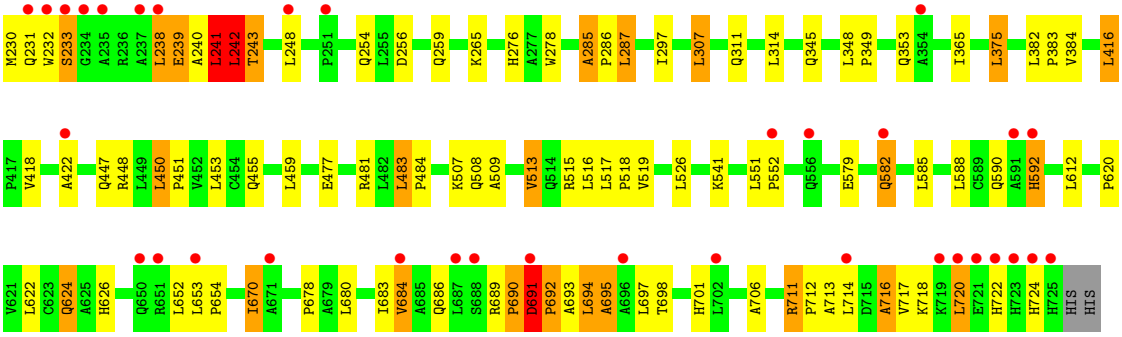




• Molecule 1: TAL effector

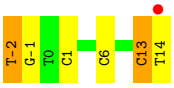
Chain B:





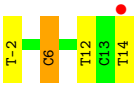
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*CP*T)-3')

Chain I:



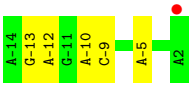
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5CM)P*GP*CP*GP*TP*CP*TP*CP*T)-3')

Chain C:



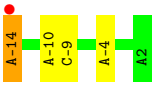
• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain J:



• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.79Å 87.38Å 88.46Å 90.00° 104.23° 90.00°	Depositor
Resolution (Å)	85.74 – 2.49 37.59 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (85.74-2.49) 98.7 (37.59-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.229 , 0.278 0.229 , 0.276	Depositor DCC
R_{free} test set	2234 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.55	0/3661	0.73	3/5001 (0.1%)
1	B	0.54	0/3655	0.79	5/4993 (0.1%)
2	C	0.54	0/349	1.04	2/533 (0.4%)
2	I	0.52	0/349	1.06	4/533 (0.8%)
3	D	0.50	0/402	0.91	2/620 (0.3%)
3	J	0.53	0/402	0.84	0/620
All	All	0.54	0/8818	0.80	16/12300 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	242	LEU	CA-CB-CG	6.86	131.09	115.30
1	B	720	LEU	CA-CB-CG	6.31	129.82	115.30
2	C	-2	DT	C5'-C4'-C3'	6.20	125.25	114.10
3	D	-14	DA	O4'-C4'-C3'	6.15	109.69	106.00
2	C	-2	DT	C5'-C4'-O4'	5.96	120.61	109.30
2	I	-2	DT	C5'-C4'-O4'	5.94	120.59	109.30
1	A	694	LEU	CA-CB-CG	5.47	127.87	115.30
1	B	241	LEU	CB-CG-CD2	5.42	120.21	111.00
3	D	-14	DA	C5'-C4'-O4'	5.32	119.40	109.30
2	I	-2	DT	O4'-C4'-C3'	5.30	109.18	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	ASP	CB-CG-OD1	5.28	123.06	118.30
2	I	13	DC	C1'-O4'-C4'	-5.20	104.91	110.10
2	I	1	DC	C1'-O4'-C4'	-5.15	104.95	110.10
1	B	481	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	369	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	481	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	692	PRO	Peptide
1	B	716	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3606	0	3740	59	0
1	B	3601	0	3735	95	0
2	C	336	0	195	14	0
2	I	336	0	195	14	0
3	D	355	0	189	3	0
3	J	355	0	189	3	0
4	A	24	0	0	1	0
4	B	9	0	0	0	0
4	C	5	0	0	1	0
4	D	1	0	0	0	0
4	I	4	0	0	0	0
All	All	8632	0	8243	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ARG:CZ	2:C:12:DT:P	2.11	1.38
1:B:711:ARG:NE	2:C:12:DT:OP1	1.57	1.32
1:B:711:ARG:CZ	2:C:12:DT:OP2	1.81	1.24
1:B:711:ARG:NH2	2:C:12:DT:P	2.22	1.12
1:B:711:ARG:NH1	2:C:12:DT:OP2	1.85	1.09
1:B:711:ARG:NH2	2:C:12:DT:OP2	1.87	1.06
1:B:711:ARG:CZ	1:B:712:PRO:HD3	2.00	0.92
1:B:711:ARG:CZ	2:C:12:DT:OP1	2.12	0.89
1:B:652:LEU:HD13	1:B:684:VAL:HG21	1.55	0.89
1:B:689:ARG:O	1:B:691:ASP:N	2.07	0.87
1:B:711:ARG:CD	2:C:12:DT:OP1	2.25	0.85
2:I:13:DC:H2"	2:I:14:DT:O5'	1.79	0.82
1:B:241:LEU:HD22	1:B:242:LEU:N	1.93	0.81
1:B:686:GLN:O	1:B:690:PRO:HA	1.84	0.76
1:B:588:LEU:O	1:B:592:HIS:O	2.04	0.75
1:B:652:LEU:HD13	1:B:684:VAL:CG2	2.15	0.74
1:B:711:ARG:NE	1:B:712:PRO:HD3	2.01	0.74
2:I:13:DC:H1'	2:I:14:DT:H5'	1.71	0.72
1:A:691:ASP:HB3	1:A:692:PRO:HD2	1.72	0.71
2:I:14:DT:OP1	1:B:720:LEU:HB3	1.91	0.71
2:I:14:DT:P	1:B:720:LEU:HB3	2.31	0.70
1:B:694:LEU:HG	1:B:695:ALA:N	2.08	0.69
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.23	0.69
1:B:232:TRP:O	1:B:233:SER:HB2	1.91	0.69
1:B:265:LYS:HE3	3:D:-4:DA:OP2	1.91	0.69
1:B:240:ALA:O	1:B:243:THR:HG23	1.93	0.69
1:A:701:HIS:HA	1:B:701:HIS:CE1	2.28	0.69
1:B:711:ARG:NH2	2:C:12:DT:O5'	2.24	0.69
1:B:691:ASP:HB3	1:B:692:PRO:HD3	1.74	0.68
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.25	0.67
1:B:692:PRO:O	1:B:694:LEU:N	2.28	0.67
2:I:13:DC:C1'	2:I:14:DT:H5'	2.25	0.66
1:A:701:HIS:CE1	1:B:701:HIS:CD2	2.85	0.65
1:B:691:ASP:HB3	1:B:692:PRO:CD	2.29	0.63
1:B:241:LEU:HD22	1:B:241:LEU:C	2.19	0.62
2:I:13:DC:H1'	2:I:14:DT:C5'	2.32	0.58
1:A:270:THR:HG23	2:I:-1:DG:OP1	2.03	0.58
1:A:493:THR:HG23	1:A:496:GLN:HG3	1.86	0.57
1:B:691:ASP:O	1:B:692:PRO:C	2.43	0.56
1:A:626:HIS:HB3	1:A:653:LEU:HD23	1.87	0.56
1:A:262:LYS:HE3	3:J:-5:DA:OP1	2.05	0.56
1:A:708:LEU:HD21	1:B:695:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:TRP:O	1:B:233:SER:CB	2.54	0.56
1:B:711:ARG:CZ	1:B:712:PRO:CD	2.81	0.56
1:B:626:HIS:HB3	1:B:653:LEU:HD23	1.87	0.55
1:A:285:ALA:CB	1:A:286:PRO:CD	2.85	0.54
2:I:13:DC:O2	1:B:724:HIS:CD2	2.61	0.54
1:B:241:LEU:C	1:B:243:THR:N	2.60	0.54
1:B:692:PRO:C	1:B:694:LEU:N	2.61	0.54
1:A:508:GLN:HB3	1:A:541:LYS:HD3	1.90	0.53
1:B:670:ILE:HD13	1:B:706:ALA:HB3	1.89	0.53
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.91	0.52
1:A:517:LEU:N	1:A:518:PRO:HD2	2.24	0.52
1:B:680:LEU:O	1:B:684:VAL:HG23	2.10	0.52
1:B:285:ALA:CB	1:B:286:PRO:CD	2.88	0.52
1:B:678:PRO:HB2	1:B:711:ARG:HD3	1.92	0.52
2:I:14:DT:OP1	1:B:720:LEU:C	2.49	0.51
1:B:620:PRO:O	1:B:624:GLN:HG2	2.11	0.51
2:I:13:DC:N1	2:I:14:DT:H5'	2.26	0.50
1:B:416:LEU:O	1:B:416:LEU:HD13	2.11	0.50
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.92	0.50
1:A:495:GLN:HG3	4:A:805:HOH:O	2.11	0.49
1:B:241:LEU:C	1:B:241:LEU:CD2	2.77	0.49
1:B:517:LEU:N	1:B:518:PRO:HD2	2.27	0.49
1:B:711:ARG:HD2	2:C:12:DT:OP1	2.12	0.49
1:A:416:LEU:HD13	1:A:416:LEU:O	2.13	0.49
1:A:694:LEU:HD13	1:A:695:ALA:HB2	1.94	0.49
1:B:450:LEU:C	1:B:450:LEU:HD13	2.33	0.49
1:B:508:GLN:HB3	1:B:541:LYS:HD3	1.94	0.49
1:A:579:GLU:O	1:A:582:GLN:HB3	2.13	0.49
1:A:287:LEU:HD21	1:A:311:GLN:HA	1.95	0.48
1:A:297:ILE:HG22	1:A:307:LEU:HD13	1.95	0.48
1:A:721:GLU:HG2	1:A:725:HIS:HB3	1.96	0.48
1:B:418:VAL:O	1:B:422:ALA:HB3	2.14	0.48
1:A:708:LEU:HD11	1:B:695:ALA:HB2	1.96	0.48
1:A:670:ILE:HD13	1:A:706:ALA:HB3	1.96	0.47
1:A:689:ARG:O	1:A:690:PRO:C	2.50	0.47
1:B:297:ILE:HG22	1:B:307:LEU:HD13	1.96	0.47
1:A:231:GLN:C	1:A:233:SER:H	2.17	0.47
1:A:418:VAL:O	1:A:422:ALA:HB3	2.14	0.47
1:B:241:LEU:C	1:B:243:THR:H	2.18	0.47
1:B:579:GLU:O	1:B:582:GLN:HB3	2.14	0.47
1:B:711:ARG:NE	2:C:12:DT:P	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:LEU:CD1	1:B:684:VAL:HG21	2.37	0.47
1:A:365:ILE:HG22	1:A:375:LEU:HD13	1.97	0.47
2:I:13:DC:C2	2:I:14:DT:H5'	2.49	0.46
1:B:287:LEU:HD21	1:B:311:GLN:HA	1.98	0.46
1:B:451:PRO:O	1:B:455:GLN:HG2	2.16	0.46
1:B:240:ALA:O	1:B:242:LEU:N	2.49	0.46
1:A:231:GLN:HB2	1:A:233:SER:H	1.81	0.46
1:B:365:ILE:HG22	1:B:375:LEU:HD13	1.98	0.46
1:A:231:GLN:NE2	2:I:-2:DT:O5'	2.48	0.45
1:A:656:LEU:HD21	1:A:684:VAL:HG23	1.97	0.45
1:A:708:LEU:HD11	1:B:695:ALA:CB	2.47	0.45
1:B:694:LEU:O	1:B:695:ALA:HB2	2.16	0.45
1:A:416:LEU:HD13	1:A:416:LEU:C	2.36	0.45
3:J:-10:DA:H2'	3:J:-9:DC:C6	2.52	0.45
1:B:382:LEU:N	1:B:383:PRO:CD	2.80	0.45
1:A:516:LEU:HA	1:A:519:VAL:HG12	1.98	0.45
1:B:314:LEU:C	1:B:314:LEU:HD23	2.38	0.44
2:I:14:DT:OP1	1:B:720:LEU:O	2.35	0.44
1:B:516:LEU:HA	1:B:519:VAL:HG12	2.00	0.44
1:A:478:THR:OG1	1:A:507:LYS:HG2	2.18	0.44
1:A:232:TRP:O	1:A:232:TRP:CG	2.71	0.43
1:B:416:LEU:HD13	1:B:416:LEU:C	2.38	0.43
1:A:720:LEU:CD1	1:B:713:ALA:HA	2.48	0.43
1:A:293:GLN:HE21	1:A:326:GLN:NE2	2.16	0.43
1:A:701:HIS:CD2	1:B:701:HIS:HA	2.53	0.43
3:J:-13:DG:H2"	3:J:-12:DA:C8	2.54	0.43
1:B:551:LEU:HB3	1:B:552:PRO:HD3	2.01	0.43
1:B:620:PRO:O	1:B:624:GLN:CG	2.66	0.43
1:A:701:HIS:ND1	1:B:701:HIS:NE2	2.66	0.43
1:B:256:ASP:OD1	1:B:259:GLN:HG3	2.19	0.43
1:B:483:LEU:N	1:B:484:PRO:HD2	2.34	0.43
1:A:513:VAL:O	1:A:515:ARG:O	2.37	0.43
1:B:513:VAL:O	1:B:517:LEU:HB2	2.19	0.43
1:B:698:THR:OG1	1:B:701:HIS:CD2	2.72	0.43
1:B:248:LEU:HD21	1:B:276:HIS:HA	2.00	0.43
1:A:483:LEU:N	1:A:484:PRO:HD2	2.34	0.42
1:B:448:ARG:NH2	1:B:477:GLU:OE2	2.52	0.42
1:B:711:ARG:N	1:B:712:PRO:CD	2.82	0.42
1:A:314:LEU:C	1:A:314:LEU:HD23	2.40	0.42
1:A:348:LEU:N	1:A:349:PRO:HD2	2.34	0.42
1:B:231:GLN:O	1:B:238:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:N	1:B:349:PRO:HD2	2.35	0.42
1:B:450:LEU:HB3	1:B:451:PRO:HD3	2.02	0.42
1:A:721:GLU:HG2	1:A:725:HIS:CB	2.49	0.42
1:B:694:LEU:O	1:B:695:ALA:CB	2.68	0.42
1:A:701:HIS:CE1	1:B:701:HIS:NE2	2.87	0.42
1:A:719:LYS:HD3	2:C:14:DT:C5	2.55	0.42
1:A:416:LEU:C	1:A:416:LEU:CD1	2.87	0.42
1:A:248:LEU:HD21	1:A:276:HIS:HA	2.02	0.41
1:B:231:GLN:O	1:B:238:LEU:HD21	2.18	0.41
3:D:-10:DA:H2'	3:D:-9:DC:C6	2.55	0.41
1:A:551:LEU:HB3	1:A:552:PRO:HD3	2.01	0.41
1:B:230:MET:HA	1:B:239:GLU:HB2	2.02	0.41
2:I:13:DC:C2'	2:I:14:DT:O5'	2.58	0.41
1:A:725:HIS:O	3:D:-14:DA:N7	2.54	0.41
1:A:514:GLN:C	1:A:515:ARG:O	2.56	0.41
1:A:689:ARG:O	1:A:691:ASP:N	2.53	0.41
1:A:711:ARG:N	1:A:712:PRO:CD	2.84	0.41
1:B:695:ALA:HB3	1:B:697:LEU:HD23	2.03	0.41
1:A:509:ALA:O	1:A:513:VAL:HG13	2.21	0.41
1:A:555:CYS:HA	1:A:560:LEU:O	2.20	0.41
1:A:705:LEU:HD21	1:A:717:VAL:HG21	2.02	0.41
1:B:509:ALA:O	1:B:513:VAL:HG13	2.21	0.41
1:B:513:VAL:O	1:B:515:ARG:O	2.37	0.41
1:B:711:ARG:NH2	1:B:712:PRO:CG	2.84	0.41
1:A:297:ILE:CG2	1:A:307:LEU:HD13	2.52	0.40
1:B:239:GLU:HA	1:B:241:LEU:HD12	2.03	0.40
1:B:653:LEU:HB3	1:B:654:PRO:HD3	2.03	0.40
1:A:382:LEU:N	1:A:383:PRO:CD	2.84	0.40
1:B:416:LEU:C	1:B:416:LEU:CD1	2.90	0.40
2:C:6:5CM:H5A1	4:C:103:HOH:O	2.21	0.40
1:A:416:LEU:HB3	1:A:417:PRO:HD3	2.02	0.40
1:A:719:LYS:HG2	2:C:14:DT:C5	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	494/498 (99%)	459 (93%)	32 (6%)	3 (1%)	25 43
1	B	494/498 (99%)	455 (92%)	27 (6%)	12 (2%)	6 9
All	All	988/996 (99%)	914 (92%)	59 (6%)	15 (2%)	10 18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	B	241	LEU
1	B	242	LEU
1	B	285	ALA
1	B	691	ASP
1	B	693	ALA
1	B	695	ALA
1	B	717	VAL
1	B	233	SER
1	B	690	PRO
1	A	690	PRO
1	B	238	LEU
1	A	695	ALA
1	B	716	ALA
1	B	718	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	380/384 (99%)	346 (91%)	34 (9%)	9 19
1	B	379/384 (99%)	344 (91%)	35 (9%)	9 18
All	All	759/768 (99%)	690 (91%)	69 (9%)	9 18

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	233	SER
1	A	238	LEU
1	A	254	GLN
1	A	278	TRP
1	A	287	LEU
1	A	307	LEU
1	A	345	GLN
1	A	353	GLN
1	A	375	LEU
1	A	384	VAL
1	A	416	LEU
1	A	447	GLN
1	A	481	ARG
1	A	483	LEU
1	A	493	THR
1	A	507	LYS
1	A	513	VAL
1	A	522	GLN
1	A	526	LEU
1	A	582	GLN
1	A	585	LEU
1	A	588	LEU
1	A	622	LEU
1	A	665	GLN
1	A	670	ILE
1	A	683	ILE
1	A	684	VAL
1	A	694	LEU
1	A	701	HIS
1	A	711	ARG
1	A	714	LEU
1	A	719	LYS
1	A	722	HIS
1	B	239	GLU
1	B	241	LEU
1	B	243	THR
1	B	254	GLN
1	B	278	TRP
1	B	287	LEU
1	B	307	LEU
1	B	345	GLN

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	375	LEU
1	B	384	VAL
1	B	416	LEU
1	B	447	GLN
1	B	450	LEU
1	B	453	LEU
1	B	459	LEU
1	B	483	LEU
1	B	507	LYS
1	B	513	VAL
1	B	526	LEU
1	B	582	GLN
1	B	585	LEU
1	B	590	GLN
1	B	592	HIS
1	B	612	LEU
1	B	622	LEU
1	B	624	GLN
1	B	670	ILE
1	B	683	ILE
1	B	684	VAL
1	B	691	ASP
1	B	694	LEU
1	B	711	ARG
1	B	714	LEU
1	B	722	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	311	GLN
1	A	326	GLN
1	A	423	HIS
1	A	592	HIS
1	A	699	ASN
1	A	724	HIS
1	B	423	HIS
1	B	447	GLN
1	B	686	GLN
1	B	699	ASN

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Mol	Chain	Res	Type
1	B	701	HIS
1	B	724	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5CM	I	6	2,3	17,21,22	1.05	2 (11%)	24,30,33	1.24	2 (8%)
2	5CM	C	6	2,3	17,21,22	1.07	2 (11%)	24,30,33	1.25	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5CM	I	6	2,3	-	0/7/21/22	0/2/2/2
2	5CM	C	6	2,3	-	0/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C6-C5	2.79	1.39	1.34
2	I	6	5CM	C6-N1	-2.61	1.33	1.38
2	I	6	5CM	C6-C5	2.57	1.38	1.34
2	C	6	5CM	C6-N1	-2.16	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	6	5CM	C5A-C5-C6	-3.15	118.64	122.85
2	C	6	5CM	C5-C6-N1	-3.00	120.25	123.34
2	I	6	5CM	C5-C4-N3	-2.63	118.83	121.67
2	I	6	5CM	O2-C2-N3	-2.61	118.09	122.33
2	C	6	5CM	O4'-C1'-N1	2.17	111.75	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	5CM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	496/498 (99%)	0.11	23 (4%)	32	34	34, 52, 83, 159	0
1	B	496/498 (99%)	0.56	34 (6%)	16	17	34, 59, 103, 229	0
2	C	16/17 (94%)	-0.06	1 (6%)	20	21	39, 45, 98, 148	0
2	I	16/17 (94%)	-0.23	1 (6%)	20	21	37, 41, 107, 144	0
3	D	17/17 (100%)	-0.05	1 (5%)	22	23	45, 61, 100, 162	0
3	J	17/17 (100%)	-0.19	1 (5%)	22	23	41, 55, 104, 116	0
All	All	1058/1064 (99%)	0.31	61 (5%)	23	24	34, 55, 98, 229	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	32.2
1	B	233	SER	22.4
1	B	235	ALA	15.2
1	B	720	LEU	14.2
1	B	232	TRP	13.3
1	B	723	HIS	13.1
1	B	724	HIS	12.9
1	B	725	HIS	11.7
1	B	719	LYS	11.0
1	B	722	HIS	10.9
1	B	721	GLU	10.0
3	D	-14	DA	5.9
1	A	251	PRO	5.5
1	B	238	LEU	5.4
1	A	692	PRO	5.4
1	A	691	ASP	5.3
1	B	251	PRO	5.1
1	B	237	ALA	4.2
1	B	591	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	693	ALA	3.8
2	C	14	DT	3.8
1	A	232	TRP	3.7
1	B	702	LEU	3.4
1	A	522	GLN	3.3
1	B	556	GLN	3.3
1	A	708	LEU	3.3
3	J	2	DA	3.0
1	A	230	MET	3.0
1	A	690	PRO	2.9
1	B	696	ALA	2.8
1	A	705	LEU	2.8
1	A	554	LEU	2.7
1	A	725	HIS	2.7
1	A	675	GLY	2.7
1	A	520	LEU	2.6
1	A	399	ILE	2.5
2	I	14	DT	2.5
1	B	592	HIS	2.5
1	B	248	LEU	2.4
1	A	578	LEU	2.4
1	B	231	GLN	2.4
1	B	688	SER	2.3
1	A	724	HIS	2.3
1	B	552	PRO	2.3
1	A	391	LEU	2.3
1	B	687	LEU	2.3
1	B	691	ASP	2.3
1	B	714	LEU	2.3
1	B	582	GLN	2.2
1	A	550	LEU	2.2
1	A	722	HIS	2.2
1	A	231	GLN	2.2
1	B	422	ALA	2.2
1	B	684	VAL	2.2
1	B	653	LEU	2.2
1	B	354	ALA	2.1
1	B	671	ALA	2.1
1	B	650	GLN	2.1
1	A	518	PRO	2.1
1	B	651	ARG	2.1
1	A	656	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5CM	C	6	20/21	0.96	0.12	36,40,43,45	0
2	5CM	I	6	20/21	0.98	0.13	36,40,47,48	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.